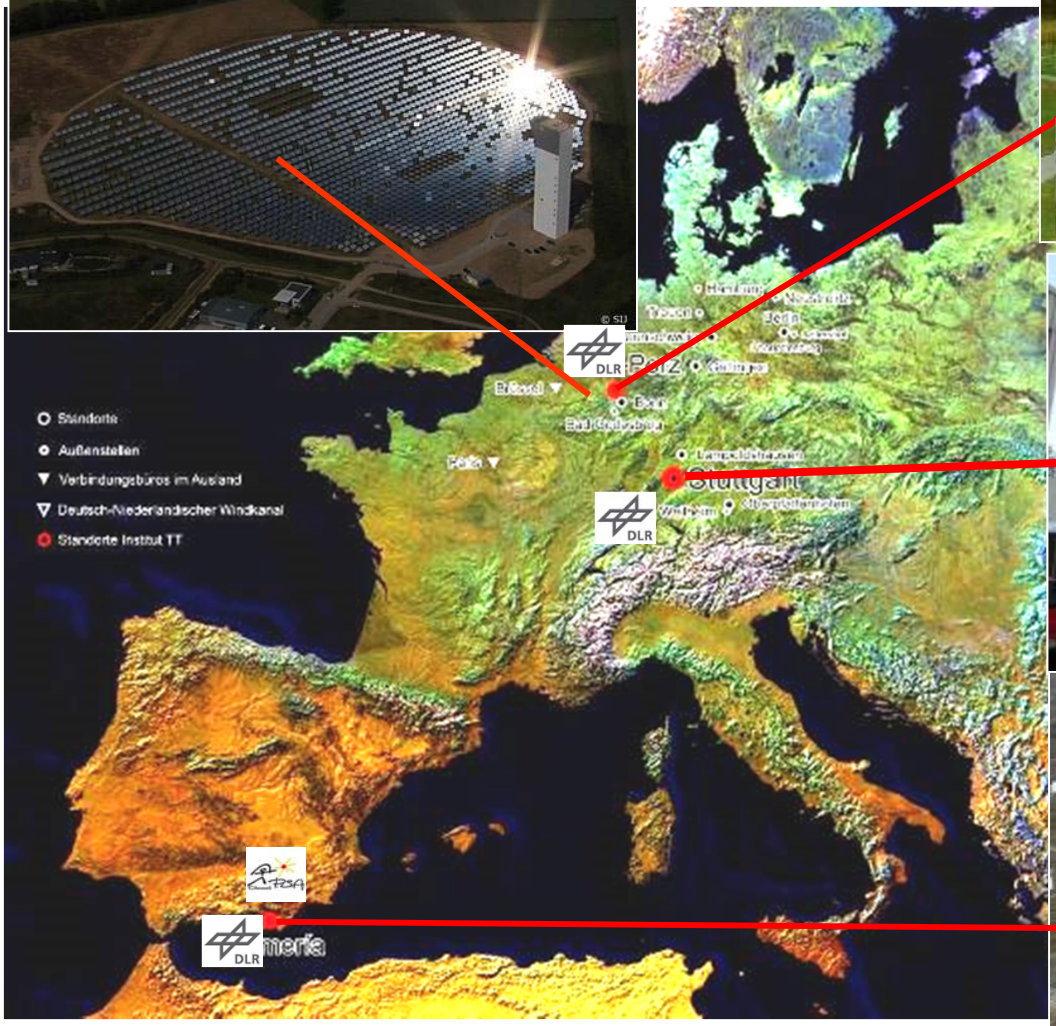
Equilibrium-Reduction of Ceria-based Materials for Solar Fuel Production

Friedemann Call[1], Martin Roeb[1], Christian Sattler[1], Martin Schmücker[2], Brendan Bulfin[3], Igor Shvets[3]

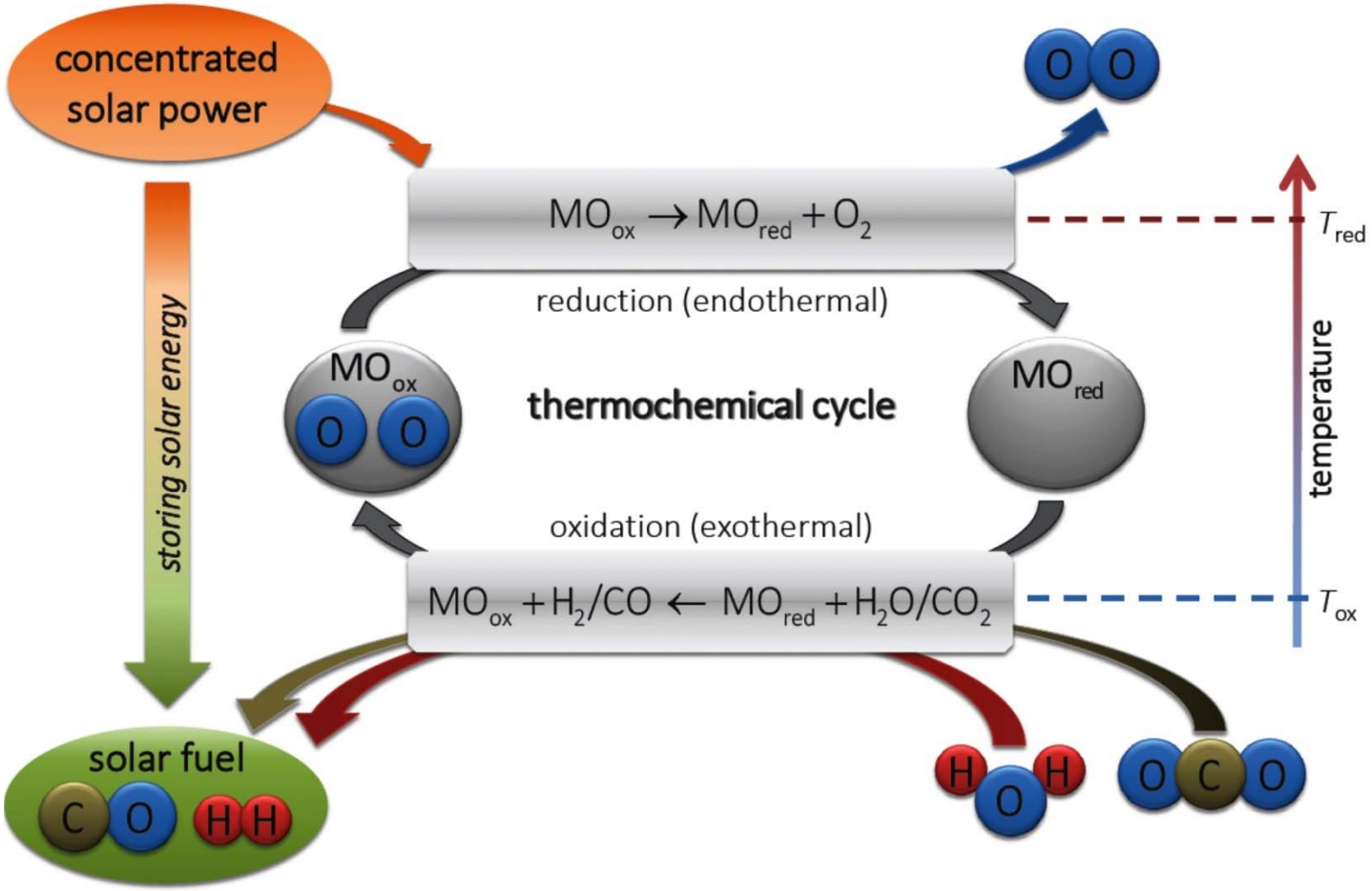
[1]Institute of Solar Research (DLR)
[2]Institute of Material Research (DLR)
[3]School of Physics, Trinity College Dublin

Institute of Solar Research

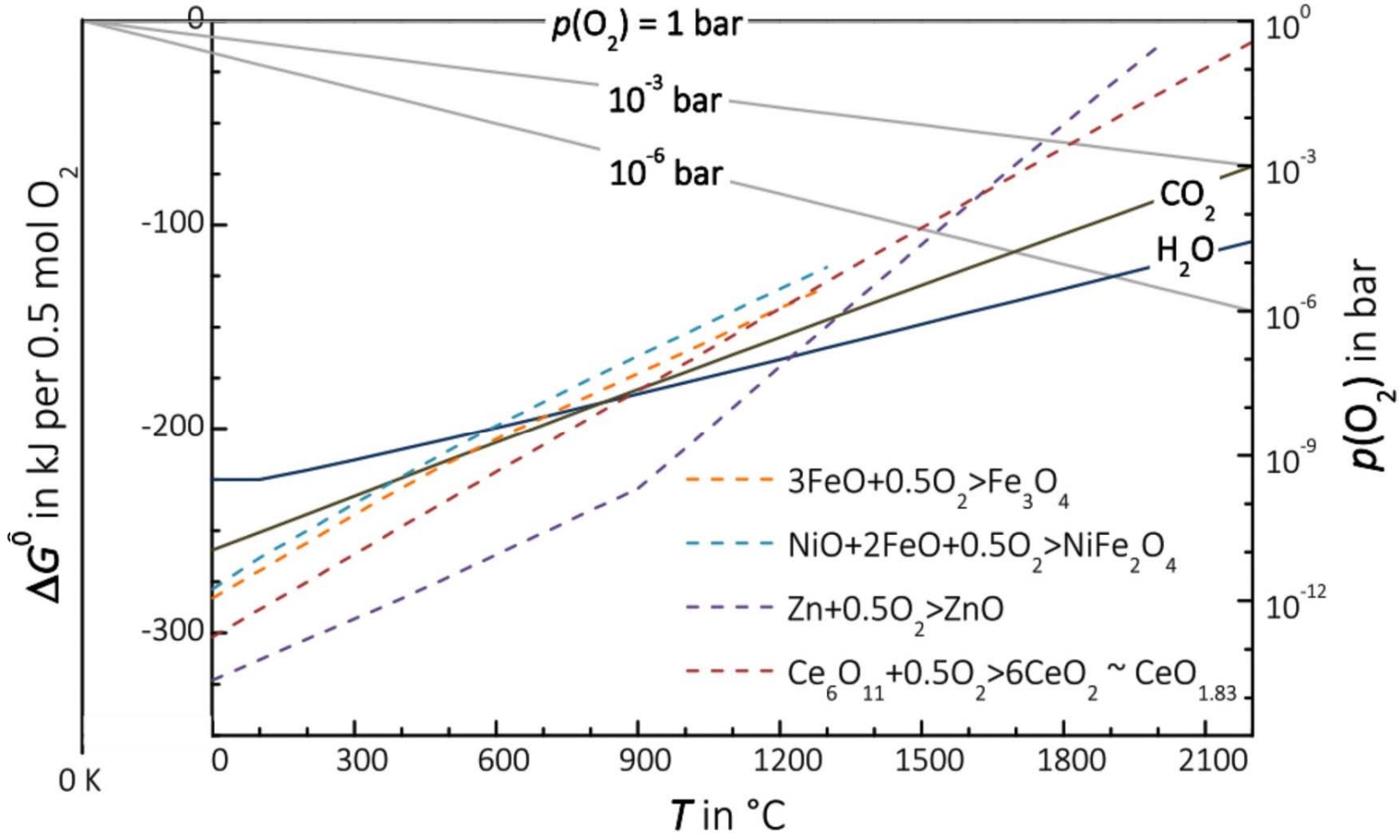


DLR

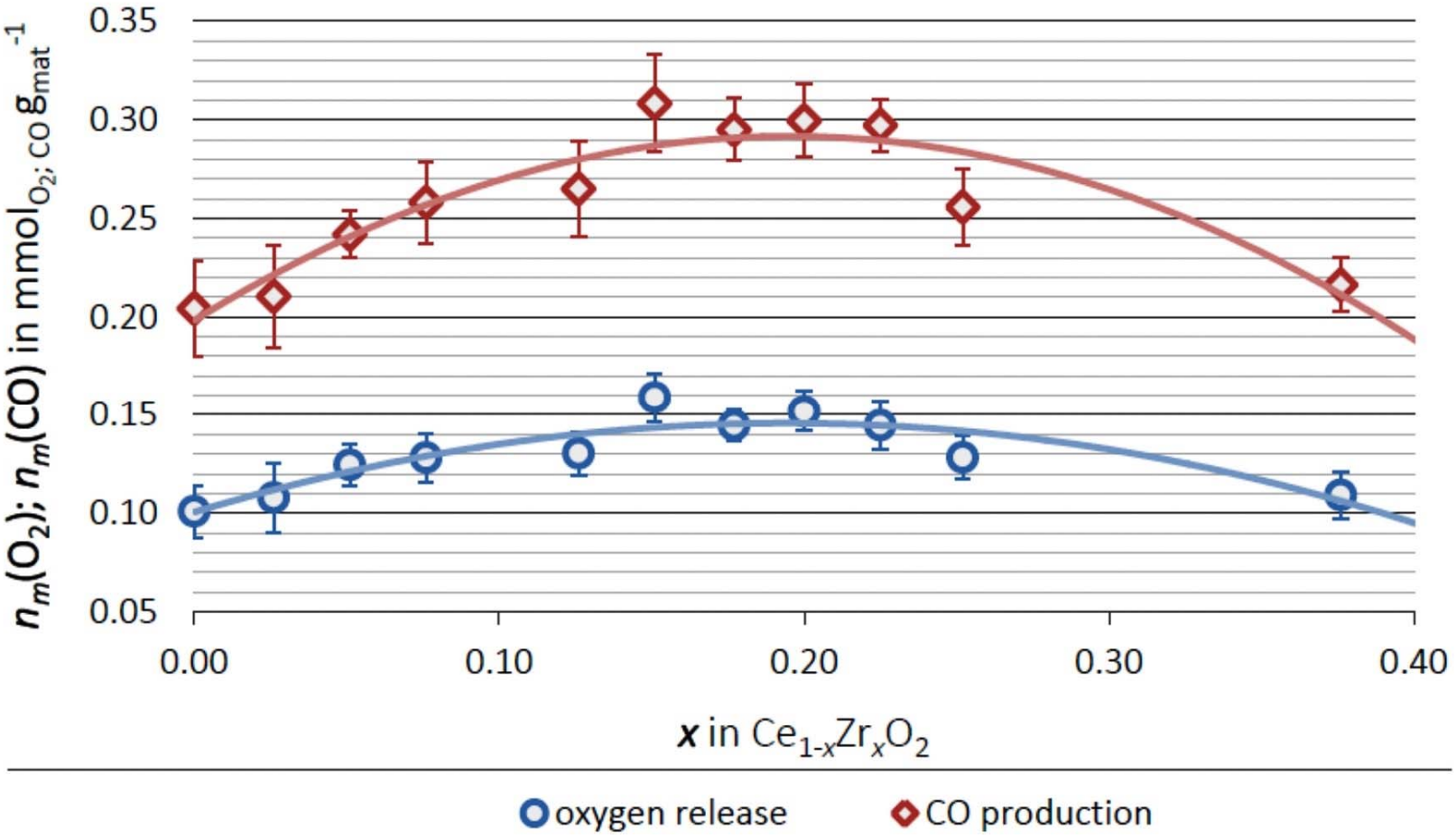
Thermochemical Redox Cycles for Synthesis Gas



The Bottle Neck: The Redox Material

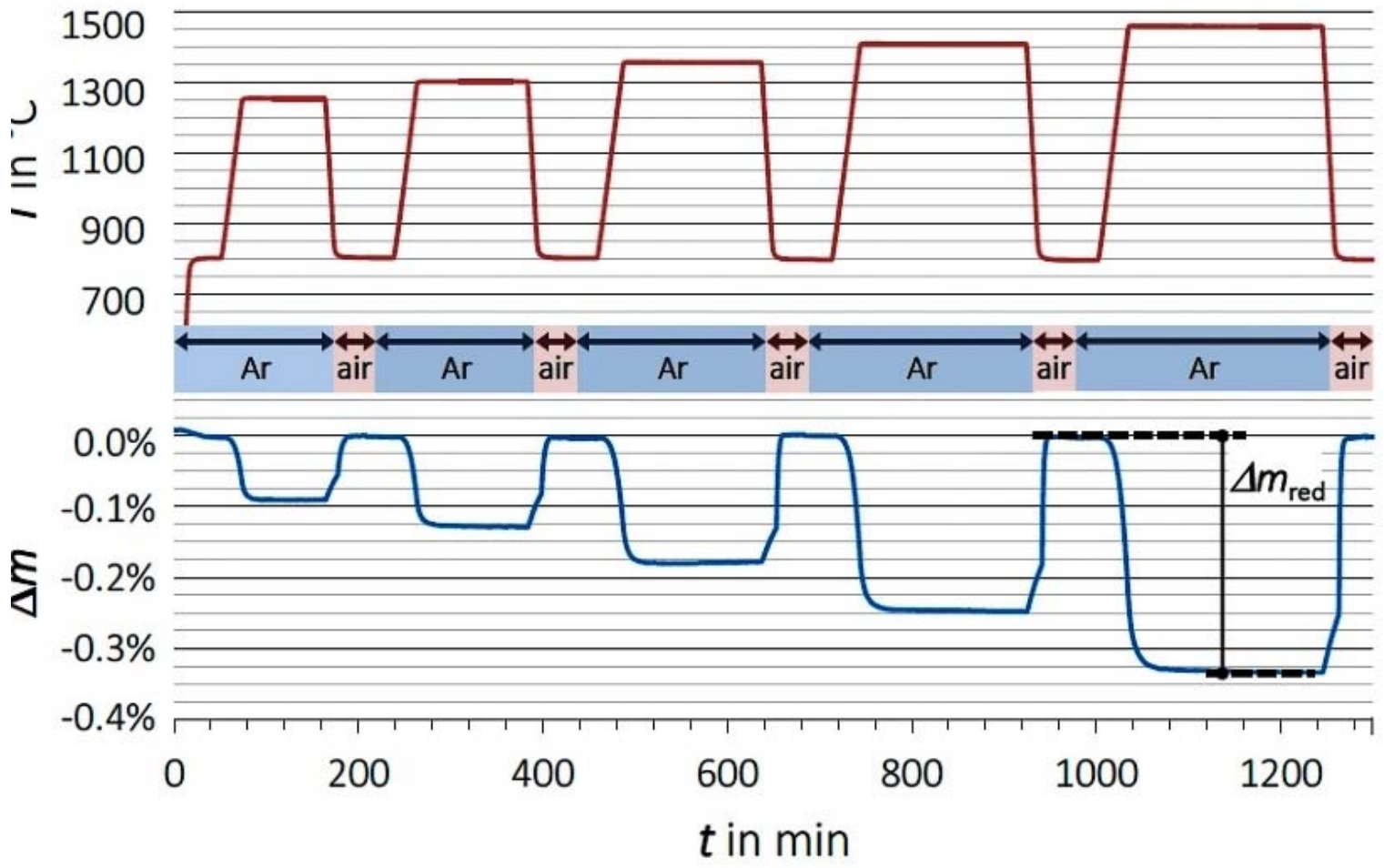


Doping Results

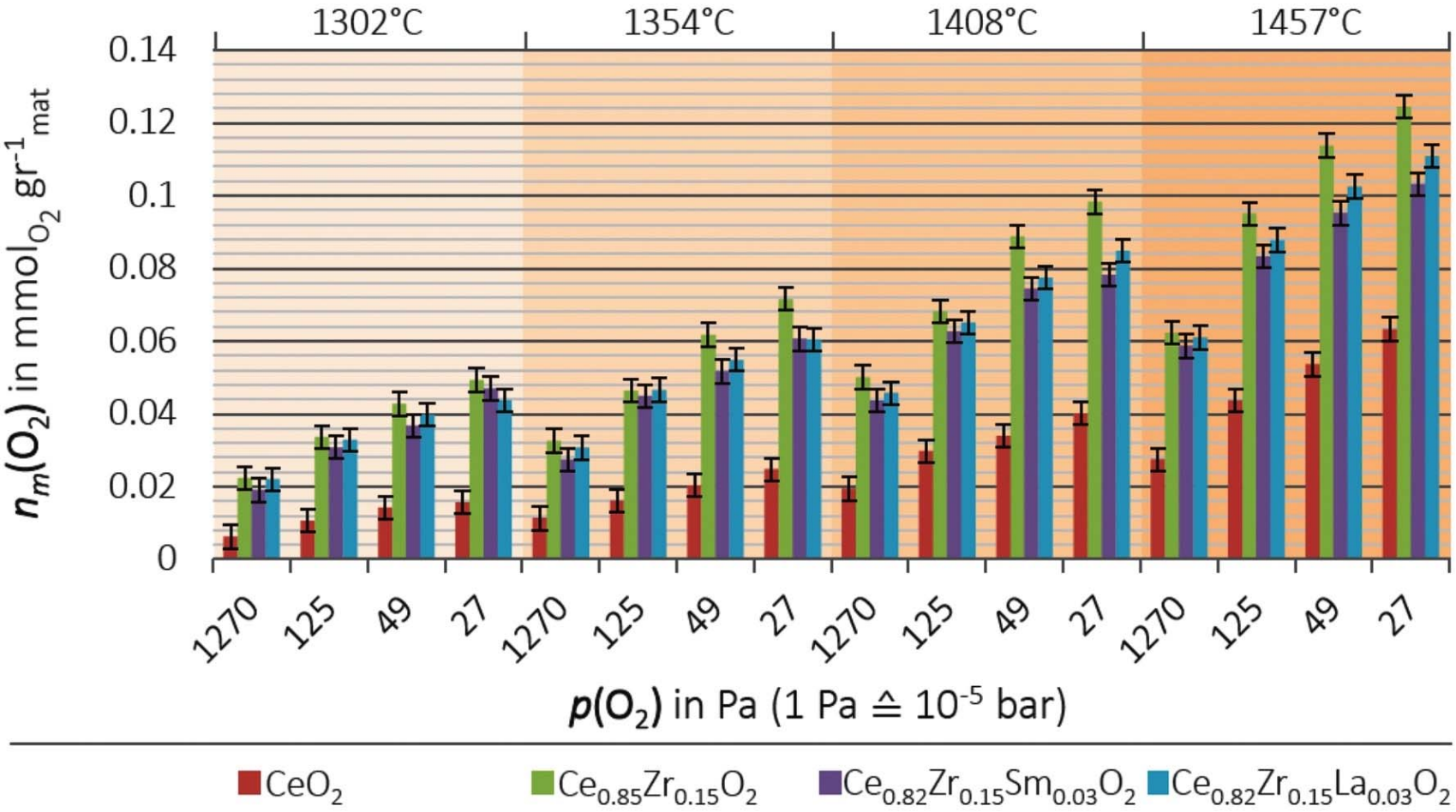


F. Call et al., The American Journal of Analytical Chemistry, Vol. 117, No. 46, pp. 24129–24137, 2013.

Reduction in Equilibrium

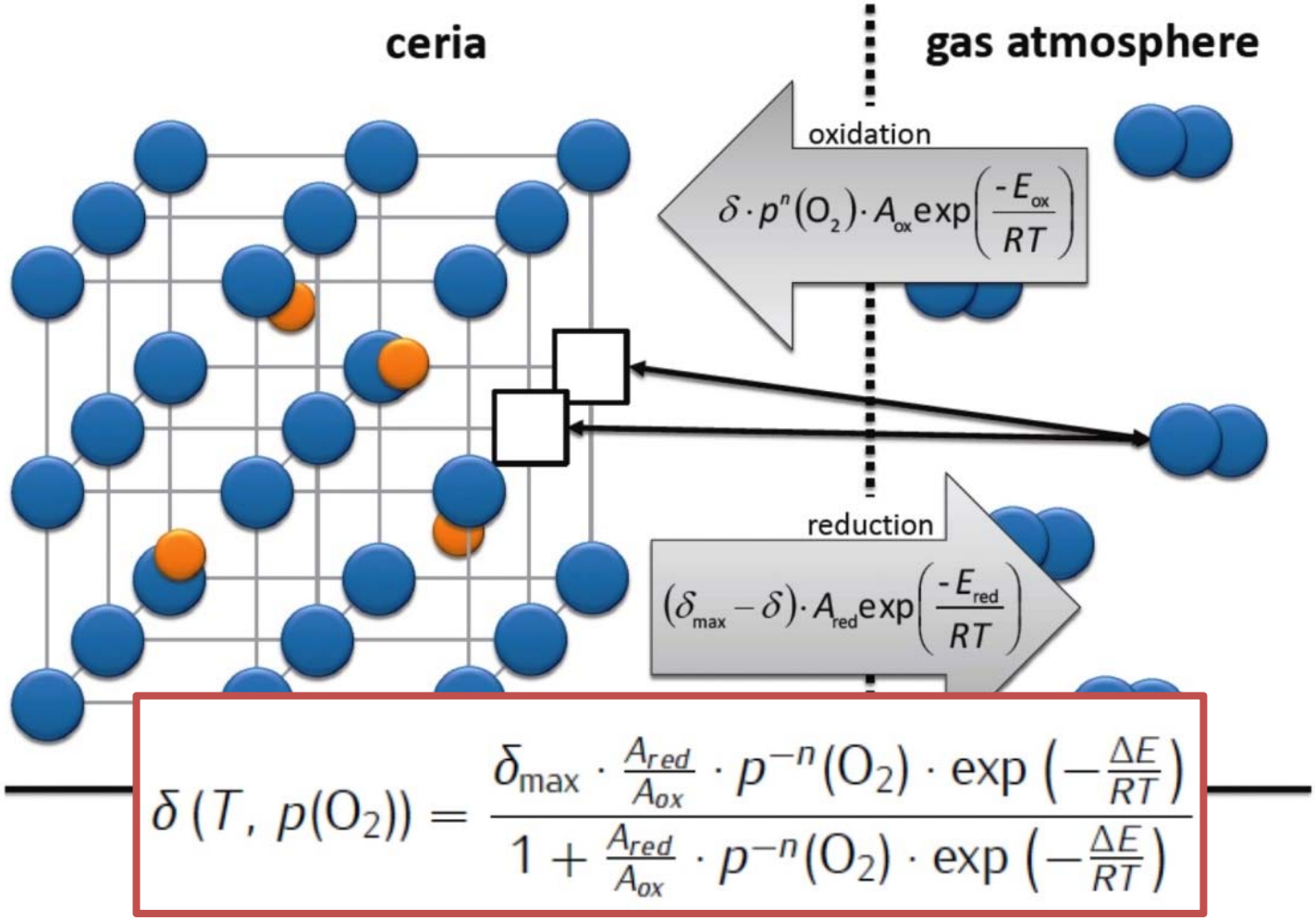


Results in Equilibirum



F. Call et al., Journal of Physical Chemistry C, under revision

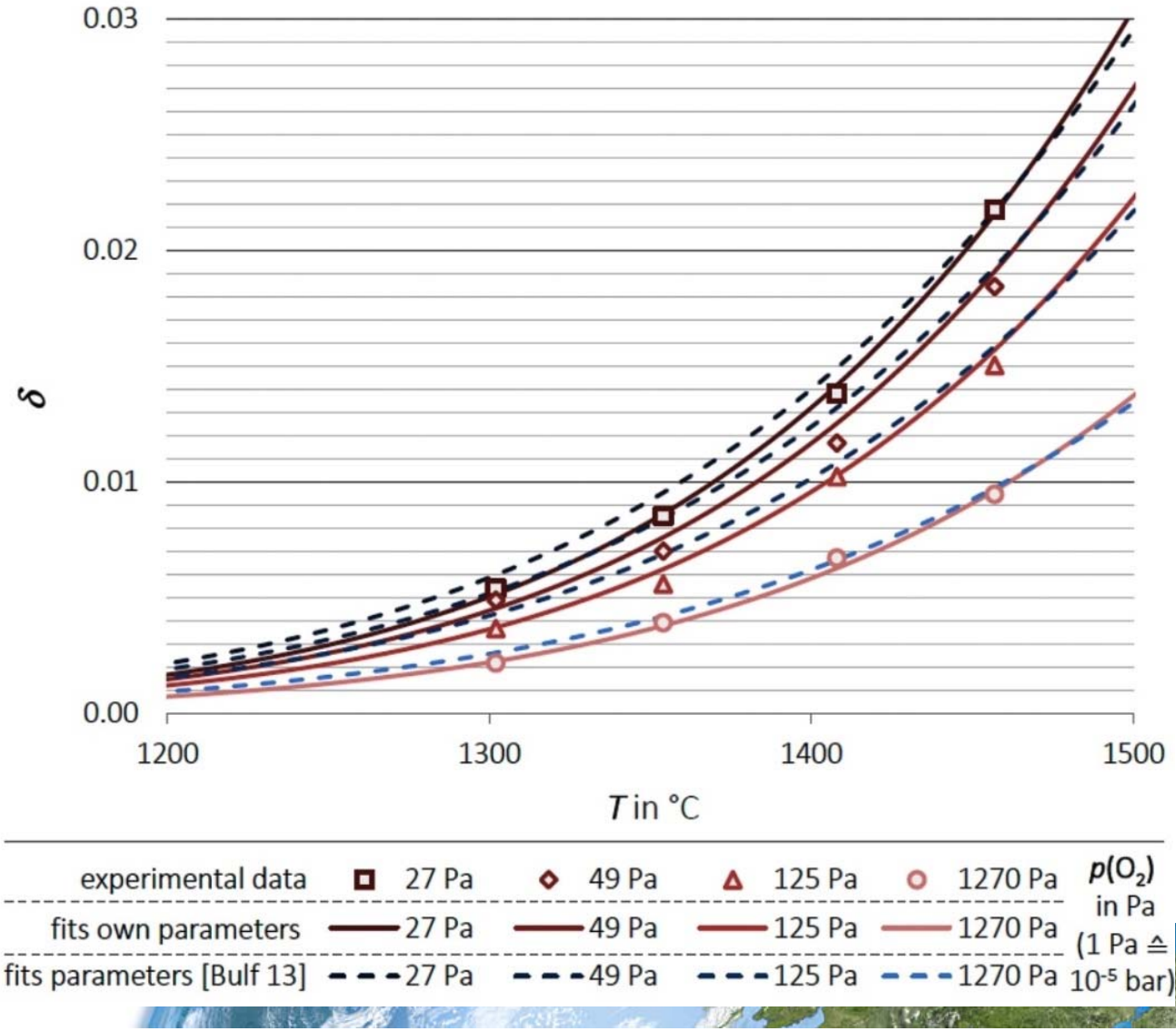
Feeding a Physical Reaction Model



$$\delta(T, p(O_2)) = \frac{\delta_{max} \cdot \frac{A_{red}}{A_{ox}} \cdot p^{-n}(O_2) \cdot \exp\left(-\frac{\Delta E}{RT}\right)}{1 + \frac{A_{red}}{A_{ox}} \cdot p^{-n}(O_2) \cdot \exp\left(-\frac{\Delta E}{RT}\right)}$$

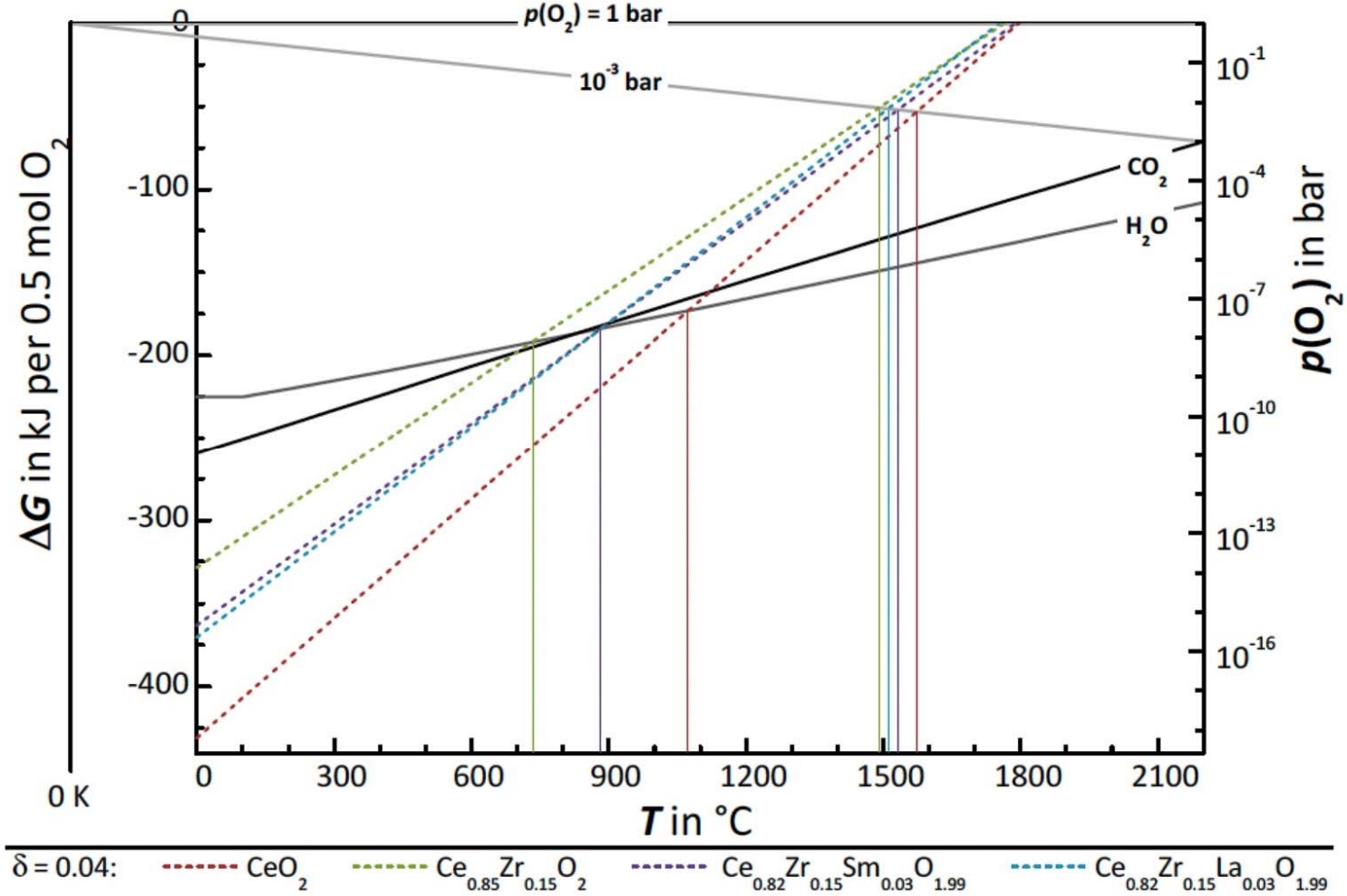
[Bul 13] B. Bulfin et al. The Journal of Physical Chemistry C, Vol. 117, No. 46, pp. 24129–24137, 2013.

Feeding a Physical Reaction Model

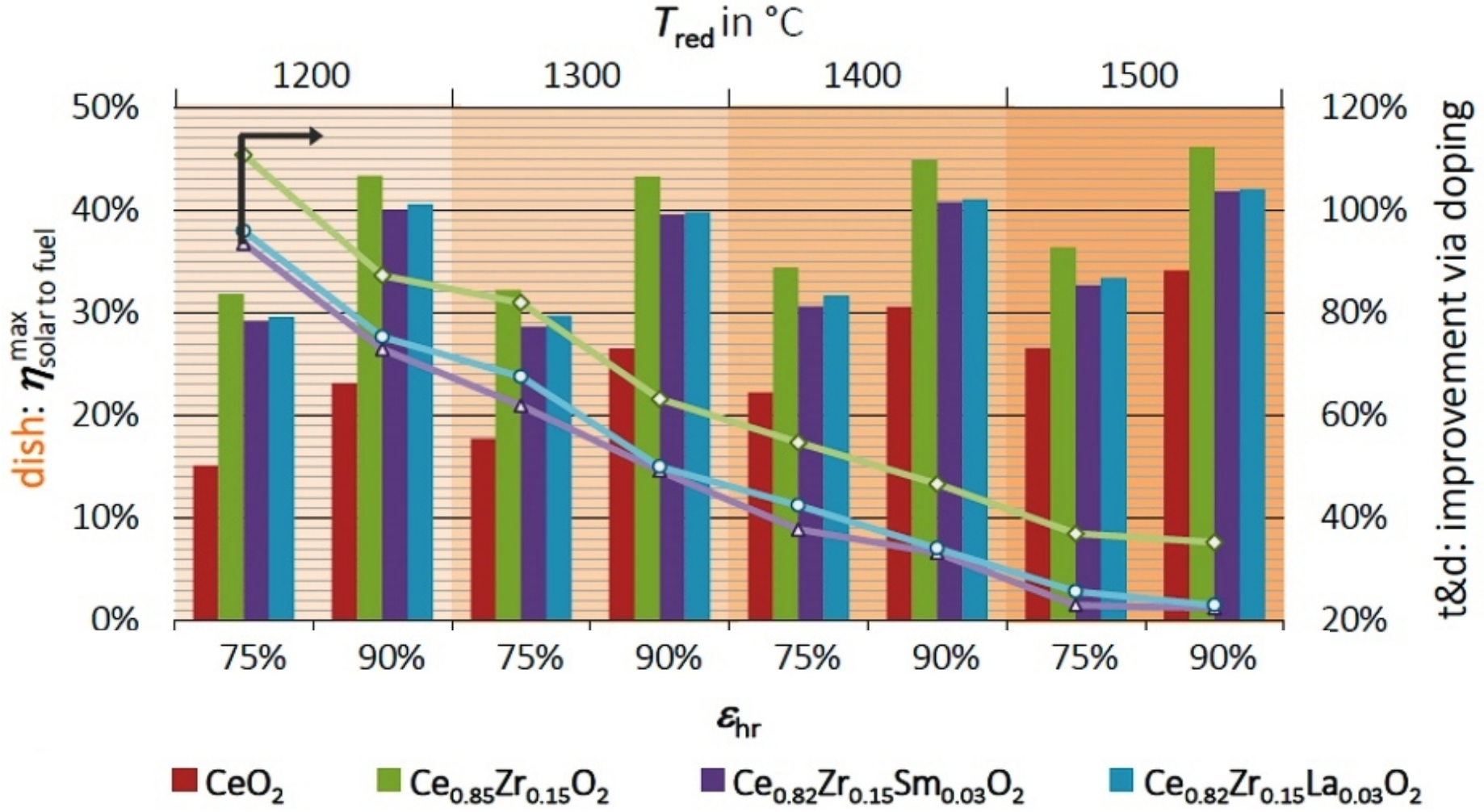


DLR

Ellingham Diagrams of Doped-Materials



Basic Efficiency Calculations



F. Call et al., PhD Thesis. Will be submitted next month.

DLR

New Idea: Ammonia Production

H_2 ✓

from water

N_2

from air

NH_3 ✓

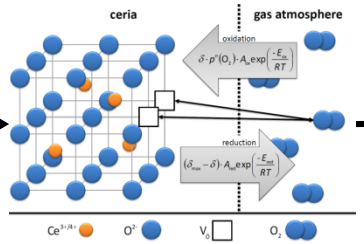
DLR

Conclusions

- Ceria-based materials are the most promising materials for Solar Fuels
- Doping yields significant improvements

- Data of equilibrium measurements (varying T and $p(O_2)$) can feed physical reaction model yielding a $\delta(T, p(O_2))$-function that can be used to construct Ellingham diagrams (reduction enthalpy and entropy)

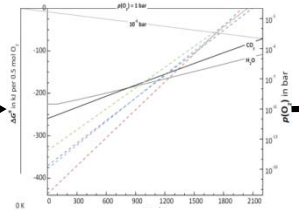
TGA



reaction model

$\delta(T, p(O_2))$

δ-function



Ellingham

$\Delta H(\delta)$

ΔH-function

- New idea: Using a combined thermochemical cycle to produce H_2 and N_2, the precursor for Ammonia

Thank you for your attention!